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An unquenched lattice QCD calculation of the mass of the bottom quark

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Abstract

We compute the b quark mass from dynamical lattice QCD with clover quarks. The calculation is done at a fixed lattice spacing with sea quark masses as low as half the strange quark mass. Our final result is $\overline{m_b}(\overline{m_b}) = 4.25(2)(11)$ GeV, where the first error is statistical and the last error is the systematic uncertainty.

1 Introduction

The mass of the bottom quark is a fundamental parameter of the standard model [1]. To extract the b mass from experiment, QCD corrections must be computed reliably. The best way to do this is use lattice QCD. The different methods of computing the mass of the bottom quark have recently been reviewed by El-Khadra and Luke [2].

The particle data table quotes the mass of the b quark in the \overline{MS} scheme at the b mass to lie between 4.0 and 4.5 GeV [3]. It is particularly important to reduce the error on the b quark mass, because it is the cause of the largest uncertainty on the determination of V_{ub} from the total inclusive B meson decay $b \to ul\nu$. El-Khadra and Luke [2] note that a 100 MeV error on m_b corresponds to a 6 % error on the V_{ub} CKM matrix element (currently only known to 19 % accuracy [3]).

In this paper we use unquenched lattice QCD with static-light mesons to extract m_b . As we discuss in section 4, the error due to the use of static (leading order HQET) approximation is only of order 30 MeV [4], hence the static limit has an important role for the phenomenology of determining V_{ub} .

2 Details of lattice calculations

We used non-perturbatively improved clover fermions in both the sea and valence quarks. The Wilson gauge action is used for the gluons. The full details of

Name	No.	$r_0 m_{PS}$	κ_{sea}	κ_{val}	Volume	$a\mathcal{E}$	$\Lambda_{static} \; \mathrm{GeV}$
DF1	20	1.92(4)	0.1395	0.1395	$12^3 \ 24$	0.87(1)	0.59(5)
DF2	78	1.94(3)	0.1395	0.1395	$16^3 \ 24$	0.842(5)	0.55(2)
DF3	60	1.93(3)	0.1350	0.1350	$16^3 \ 32$	0.772^{+7}_{-8}	0.69(7)
DF4	60	1.48(3)	0.1355	0.1355	$16^3 \ 32$	0.739_{-8}^{+9}	0.66(5)
DF5	60	1.82(3)	0.1355	0.1350	$16^3 \ 32$	0.748^{+9}_{-8}	0.68(5)
DF6	55	1.06(3)	0.1358	0.1358	$16^3 \ 32$	0.707^{+14}_{-12}	0.64(7)

Table 1: Lattice binding energy $(a\mathcal{E})$ and physical binding energy (Λ_{static}) for each data set.

the actions and details of the unquenched calculation are described in [5, 6, 7]. We use static quarks for the heavy mesons. The lattice binding energy is extracted from a two point correlator using variational smearing techniques. The local two point function is

$$C(t) = \sum_{x} \langle 0 \mid \Phi_B(x, t) \Phi_B^{\dagger}(x, 0) \mid 0 \rangle$$
 (1)

$$= Z^2 \exp(-a\mathcal{E}t) \tag{2}$$

where Φ_B is the interpolating operator for static-light mesons. We have already published [8] an extensive analysis of the spectrum of static-light mesons. Our previous paper [8] also describes the all-to-all propagators used to improve the statistical accuracy and the fuzzing methods used.

In table 1 we present our results for the lattice binding energy. All the data sets used $\beta=5.2$. Data sets DF1 and DF2 used a clover coefficient of 1.76, while all the others used the non-perturbative value of 2.0171. The results for the data sets: DF1, DF2 have already been published [8]. The ensemble size for data sets DF4 and DF5 have been trebled over the results previously published [8]. The data from ensembles DF5 and DF6 are new.

3 Extracting the quark mass

We evaluate the mass of a pseudoscalar heavy-light meson from lattice QCD with static heavy quark and compare with the experimental mass value. This gives information about the b-quark mass. The strange quark mass is accessible in lattice evaluations, so to minimise extrapolation, we use the B_s meson for this comparison. We still need to extrapolate the sea quark mass to the experimental value and we discuss this later.

In this section we will describe the central values for our calculation. We discuss systematic uncertainties in section 4. The quantity \mathcal{E} , from the lattice calculation, contains an unphysical $\frac{1}{a}$ divergence (δm) that must be subtracted

off to obtain the physical binding energy (Λ_{static}).

$$\Lambda_{static} = \mathcal{E} - \delta m \tag{3}$$

The pole quark mass is determined from

$$m_b^{pole} = M_{B_s} - \Lambda_{static} \tag{4}$$

The physical value [3] of the meson mass M_{B_s} (5.369 GeV) is used.

In the static theory δm has been calculated to two loops by Martinelli and Sachrajda [9].

$$a\delta m = 2.1173\alpha_s(\overline{m_b}) + \{(3.707 - 0.225n_f)\log(\overline{m_b}a) - 1.306 - n_f(0.104 + 0.1c_{SW} - 0.403c_{SW}^2)\}\alpha_s(\overline{m_b})^2$$
 (5)

where n_f is the number of sea quarks and c_{SW} is the coefficient of the clover term. We discuss estimates of the next order to $a\delta m$ in section 4.

The pole mass (see Kronfeld for a review [10]) is converted to \overline{MS} using continuum perturbation theory [11].

$$m_b^{\overline{MS}}(\mu) = Z_{pm}(\mu) m_b^{pole} + O(1/m_b) \tag{6}$$

where

$$Z_{pm}(\mu = m_b) = 1 - \frac{4}{3} \frac{\alpha_s(\overline{m_b})}{\pi} - (11.66 - 1.04n_f)(\frac{\alpha_s(\overline{m_b})}{\pi})^2$$
 (7)

The perturbative correction between the pole mass and the \overline{MS} mass is known to $O(\alpha^3)$ [12, 13]. The perturbative series connecting the pole mass with the \overline{MS} mass is badly behaved due to renormalons (see [14] for a review). The lattice matching is only done to $O(\alpha^2)$, hence we convert the pole mass to \overline{MS} at the same order, using a consistent coupling, so the differences in the series are physical.

We use the values of the coupling using the values of Λ_{QCD} from the joint UKQCD and QCDSF paper [15]. The four loop expression for α_s is used [16] to determine the coupling from Λ_{QCD} . We consistently use $n_f=2$ in all the perturbative expressions. For $\kappa_{sea}=0.1355$ (0.1350) we use $\Lambda_{QCD}=0.178$ (0.173) MeV [15]. We use the same value of Λ_{QCD} for the two data sets DF1 and DF2, where Λ_{QCD} has not been computed.

In [8] we estimated the mass of the strange quark using the pseudoscalar made out of strange quarks [17]. This provided $r_0m_{PS} \equiv 1.84$. This value is close to $r_0m_{PS} = 1.82^{+3}_{-1}$ for DF5 data set [6] hence we use the binding energy from that data set as the value at strange. This is a partially quenched analysis. The data sets DF1 and DF2 also have a sea quark mass close to the strange quark mass [17].

To determine the lattice spacing we use the measured value for r_0/a from the potential with the 'physical' value of r_0 as 0.525(25) fm [18]. We discuss in more detail the systematic error from the choice of r_0 in section 4. Hence our best estimate of $m_b(m_b) = 4.25(2)$ GeV from the DF5 data set, where the errors are statistical only.

4 Computing the systematic uncertainties

Gimenez et al. [4] discuss the systematic error from the neglect of the $1/m_b$ terms in the static limit. Heavy quark effective field theory parametrises the heavy mass corrections to the mass of a heavy-light meson M_B .

$$M_B = m_b + \Lambda_{static} - \frac{\lambda_1}{2m_b} - \frac{3\lambda_2}{2m_b} \tag{8}$$

where Λ_{static} is the static binding energy, λ_1 is the matrix element due to the insertion of the kinetic energy and λ_2 is the matrix element due to the insertion of the chromomagnetic operator. The value of $\lambda_2 \sim 0.12~{\rm GeV}^2$ can be obtained from the experimental mass splitting between the B^* and B mesons. The value of λ_1 is much harder to estimate. Gimenez et al. [4] use a range of λ_1 from -0.5 to 0.0 in ${\rm GeV}^2$. This includes the determination from quenched lattice QCD of $\lambda_1 = -(0.45 \pm 0.12) {\rm GeV}^2$ by Kronfeld and Simone [19]. JLQCD have recently tried to compute λ_1 using NRQCD [20]. As suggested by Gimenez et al. [4], using a symmetric error of 30 MeV to parameterise the neglected $1/m_b$ terms seems reasonable to us.

The specification of the strange quark mass, described in section 3, essentially relies on the physical K mass. Since the ϕ meson has a very narrow width, it may also be used to specify the strange quark mass. In their study using essentially the same lattice parameters, JLQCD [21] see approximately a 10% difference between using the ϕ and the K to set the strange quark mass. Motivated by JLQCD's result, we use a symmetric error of 5% as an estimate of the additional uncertainty in our estimate of the strange quark mass. This induces an error of 60 MeV in $m_b(m_b)$ for the DF5 data set.

The data sets DF1, DF2 were generated using a different value of c_{SW} to that used to generate data set DF5, hence they can not be used to estimate the size of the lattice spacing effects. The comparison of the results between data set DF1 and DF2 can in principle be used to estimate finite size effects. As the physical size of a size of the lattice changes from 1.83 fm (DF1) to 2.44 fm (DF2), $m_b(m_b)$ changes from 4.33(2) to 4.369(7) GeV. Hence, a simple estimate of the finite size effects in date set DF5 (size of box 1.77fm) is -39 MeV. In quenched QCD Duncan et al. [22] found no finite size effects in the binding energy for lattice lengths: 1.3, 1.8 and 2.2 fm. Although, finite size effects in quenched and unquenched QCD can be very different, we think it more likely that the differences in two data sets is due to a statistical fluctuation on the

smaller lattice. This is supported by the fact that UKQCD saw no finite size effects in the light hadron spectrum between DF1 and DF2 [5].

The choice of coupling is a systematic error. Gimenez et al. [4] use $\Lambda_{QCD}^{n_f=2}$ = 300 MeV as the central value. We use the result for Λ_{QCD} determined from the DF4 and DF5 data sets [15]. We don't feel that it is appropriate to use the values of Λ_{QCD} from experiment (as done by Gimenez et al. [4]) even for deriving a systematic error. The agreement between Λ_{QCD} from lattice QCD calculations and experiment is not good for calculations that use clover fermions for the sea quarks [21, 23, 15]. We assume that the discrepancy will be reduced as calculations are done with lighter sea quark masses and finer lattice spacings.

To estimate the effect of the chiral extrapolation of the sea quark masses, we extrapolated Λ_{static} from data sets DF4 and DF5 linearly in $(r_0m_{PS})^2$ to $r_0m_{PS}=1.93$ (the same as for data set DF3). The extrapolated result for Λ_{static} at $r_0m_{PS}=1.93$ at $\kappa_{sea}=0.1355$ was consistent with Λ_{static} on data set DF3 ($\kappa_{sea}=0.1350$). We see no evidence for the dependence of Λ_{static} on the sea quark mass. Gimenez et al. [4] see a slight increase in the lattice binding energy with decreasing quark mass. There are potentially non-analytic m_{PS}^3 terms in the mass dependence of the binding energy [24].

To estimate the systematic errors on the perturbative matching we did a number of things. Following Gimenez et al. [4] we compared taking the product of the two perturbative factors in equation 6 against expanding the perturbative expressions and only keeping $O(\alpha_s^2)$ terms. This increases the mass for data set DF5 by 25 MeV.

In quenched QCD the next order correction to equation 5 has been computed numerically by two groups using different techniques [25, 26]. As the two groups obtained essentially the same result we will use the result of Di Renzo and Scorzato [25]. In quenched QCD the next order correction to equation 5 is [4]

$$a\delta m^{(3)} = (\overline{X_2} + 6.48945(-3.57877 + \log(\overline{m_b}a))(3.29596 + \log(\overline{m_b}a)))\alpha_s(\overline{m_b})^3$$
(9)

where $\overline{X_2}$ is the number from the numerical calculation. Di Renzo and Scorzato [25] obtain $\overline{X_2} = 86.2(0.6)(1.0)$ for quenched QCD. Di Renzo and Scorzato have computed X_2 for $n_f = 2$ Wilson fermions [27]. The new result also involves a lattice calculation of the \overline{MS} coupling for Wilson fermions, so it is not obvious how to incorporate the new result into this analysis.

The next order to the connection between the pole mass and \overline{MS} mass is known in the continuum (equation 7).

$$Z_{pm}^{(3)} = -(157.116 - 23.8779n_f + 0.6527n_f^2)(\frac{\alpha_s(\overline{m_b})}{\pi})^3$$
 (10)

Because equation 9 is known for quenched QCD, we do not use it for our central result. It does seem appropriate to use equation 9 and equation 10 to estimate the systematic errors due to the neglect of higher order terms. We set $n_f=0$ in equation 10. Adding in the next order term reduces the mass of the bottom quark by 12 MeV for data set DF5.

Because of limitations in computer time, the unquenched calculations are at fixed lattice spacing (so the continuum limit has not been taken) and fairly heavy sea quark masses are used. This means that different lattice quantities produce slightly different values of the lattice spacing. In [18] the values of r_0 from various calculations that used clover fermions are collected together. The results were in the range $r_0 = 0.5$ to 0.55 fm. This motivates our choice of $r_0 = 0.525(25)$ fm. Using mass splittings in Upsilon on improved staggered configurations with measurements of the potential MILC [28] quote $r_0 = 0.467$ fm. This is 2.3σ from our central value for r_0 . In the graph [29] of spread of variation of lattice spacings from different physical quantities, the most dramatic failures of the quenched approximation occur for P-S and 2S-1S mass splittings in Upsilon and the pion decay constant. We speculate that these quantities are more sensitive to the heavy quark potential at the origin that depends on n_f from the running of the coupling (see [30] for a discussion of this). The relatively strong dependence of the Upsilon mass splittings and pion decay constant on the sea quark mass and lattice spacing doesn't make them a good choice to set the scale for current unquenched calculations with clover fermions. Hence we feel that using the value from MILC for r_0 (as advocated in [31]) will artificially inflate the error bars, so we stick to our original estimate of $r_0 = 0.525(25)$ fm.

The perturbative analysis, used in the this section, assumes that the sea quark mass is zero. However, the sea quark masses used in current calculations with Wilson-like quarks are not negligible. At $\kappa_{sea}=0.1355$ and 0.1350, the vector definitions of the sea quark mass (in units of the lattice spacing) are 0.026 and 0.044 respectively. The light quark mass dependence has been computed by Bali and Boyle [32].

For light quark masses below 0.1 (in lattice units) Bali and Boyle [32] provide a quadratic parameterisation of the light quark mass dependence of δm . The expression in equation 5 gets modified to

$$a\delta m = 2.1171\alpha_s(\overline{m_b}) + ((3.707 - 0.225n_f)\log(\overline{m_b}a) - 1.306 - n_f(-0.199 + 0.516m_q - 0.421m_q^2))\alpha_s(\overline{m_b})^2$$
 (11)

where we have specialised to $c_{SW}=1$. Equation 5 is a combination of the two loop static self energy and a conversion from the bare coupling to the massless \overline{MS} scheme [9]. As stressed by Martinelli and Sachrajda [9], it is important to use a consistent coupling in equation 6, so that the poorly behaved perturbative expansion of Z_{pm} cancels with that of δm . This makes it easier to use the massless quark \overline{MS} scheme. The determination of Λ_{QCD} includes the effects of the masses of the light quarks [15]. The use of 11 changes the central value of $m_b(m_b)$ by 1 MeV for the data set DF5.

For our final result we use the central value from data set DF5. The systematic uncertainties have been discussed in this section. Hence our final result is

$$\overline{m_b}(\overline{m_b}) = (4.25 \pm 0.02 \pm 0.03 \pm 0.03 \pm 0.08 \pm 0.06) \text{GeV}$$
 (12)

Group	comment	$m_b(m_b) \mathrm{GeV}$
This work	unquenched	4.25(2)(11)
Collins [35]	unquenched	$4.34(7)_{-7}^{+0}$
Gimenez et al. [4]	unquenched	4.26(9)
Di Renzo and Scorzato [4]	unquenched	$4.21 \pm 0.03 \pm 0.05 \pm 0.04$
Bali and Pineda [36]	quenched	4.19(6)(15)
Heitger and Sommer [34]	quenched	4.12(8)

Table 2: Lattice QCD results for $m_b(m_b)$ in the \overline{MS} scheme. The last error on the Bali and Pineda result is an estimate of unquenching.

where the errors are (from left to right): statistical, perturbative, and neglect of $1/m_b$ terms, ambiguities in the choice of lattice spacing, and error in the choice of the mass of the strange quark.

Gimenez et al. [4] obtain

$$\overline{m_b}(\overline{m_b}) = (4.26 \pm 0.03 \pm 0.05 \pm 0.07) \text{GeV}$$
 (13)

from a simulation at $\beta=5.6$ and volume = 24^3 40 with two dynamical quark masses, from the $T\chi L$ collaboration. The first error is due to statistics. The second error includes the neglect of the $1/m_b$ terms and the ambiguity in the determination of the lattice spacing. The third error is due to the neglect of higher order corrections in the perturbative matching. Gimenez et al. [4] used a preliminary result for $\overline{X_2}$, that was relatively imprecise [33] hence their estimate of the higher order effects is looser than ours. Also we used Λ_{QCD} determined consistently from this data set, while Gimenez et al. [4] used continuum based estimates of the coupling. This analysis has recently been updated by Di Renzo and Scorzato [27] with the unquenched value of X_2 . Gimenez et al. [4] only used one quantity to estimate the lattice spacing, so their error from the ambiguity in the choice of lattice spacing is underestimated in the final result. However, the two effects compensate and the final error is probably representative. It is pleasing that our calculation with a different set of parameters is essentially consistent with that of Gimenez et al. [4].

5 Conclusions

In table 2 we collect some recent results for the mass of the bottom quark from lattice QCD. Our result is consistent with the previous unquenched calculations. Unfortunately, we have not managed to reduce the size of the error bars. The largest error in the recent values for the mass of the bottom quark is due to the spread in different lattice spacings. Heitger and Sommer [34] noted that a change in r_0 by 10% changed the value of $m_b(m_b)$ by 150 MeV.

The prospects for an improved estimate of the mass of the bottom quark from lattice QCD are quite good. The unquenched calculations with improved

staggered quarks produce consistent lattice spacings from many different quantities [29]. The numerical calculation of the third order contribution to δm has been done for unquenched Wilson fermions [27]. Applying the technology of Heitger and Sommer [34] to unquenched calculations would allow a nonperturbative estimate of the mass of the bottom quark that is free from problems with delicate cancellations of poorly converging perturbative expressions. The use of automated perturbative calculations may allow the computation of the bottom quark mass from NRQCD / FNAL type calculations with two loop accuracy [37, 38]. We are investigating the use of the static formulation introduced by the ALPHA collaboration [39], but the required perturbative (or non-perturbative) factors are not available yet.

Some combination of the techniques and projects mentioned in the last paragraph should be able to produce a number of independent calculations, with different systematic errors, of the mass of the bottom quark from unquenched lattice QCD.

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References

- [1] V. Lubicz, Nucl. Phys. Proc. Suppl. 94, 116 (2001), hep-lat/0012003,
- [2] A. X. El-Khadra and M. Luke, Ann. Rev. Nucl. Part. Sci. 52, 201 (2002), hep-ph/0208114,
- [3] Particle Data Group, K. Hagiwara et al., Phys. Rev. **D66**, 010001 (2002),
- [4] V. Gimenez, L. Giusti, G. Martinelli, and F. Rapuano, JHEP 03, 018 (2000), hep-lat/0002007,
- [5] UKQCD, C. R. Allton et al., Phys. Rev. D60, 034507 (1999), hep-lat/9808016,
- [6] UKQCD, C. R. Allton et al., Phys. Rev. D65, 054502 (2002), hep-lat/0107021,
- [7] UKQCD, C. R. Allton et al., (2004), hep-lat/0403007,
- [8] UKQCD, A. M. Green, J. Koponen, C. McNeile, C. Michael, and G. Thompson, (2003), hep-lat/0312007,

- [9] G. Martinelli and C. T. Sachrajda, Nucl. Phys. **B559**, 429 (1999), hep-lat/9812001,
- [10] A. S. Kronfeld, Phys. Rev. **D58**, 051501 (1998), hep-ph/9805215,
- [11] N. Gray, D. J. Broadhurst, W. Grafe, and K. Schilcher, Z. Phys. C48, 673 (1990),
- [12] K. Melnikov and T. v. Ritbergen, Phys. Lett. B482, 99 (2000), hep-ph/9912391,
- [13] K. G. Chetyrkin and M. Steinhauser, Nucl. Phys. B573, 617 (2000), hep-ph/9911434,
- [14] M. Beneke, Phys. Rept. 317, 1 (1999), hep-ph/9807443,
- [15] QCDSF-UKQCD, S. Booth et al., Phys. Lett. B519, 229 (2001), hep-lat/0103023,
- [16] K. G. Chetyrkin, J. H. Kuhn, and M. Steinhauser, Comput. Phys. Commun. 133, 43 (2000), hep-ph/0004189,
- [17] UKQCD, C. McNeile and C. Michael, Phys. Lett. B491, 123 (2000), hep-lat/0006020,
- [18] UKQCD, A. Dougall, R. D. Kenway, C. M. Maynard, and C. McNeile, Phys. Lett. B569, 41 (2003), hep-lat/0307001,
- [19] A. S. Kronfeld and J. N. Simone, Phys. Lett. B490, 228 (2000), hep-ph/0006345,
- [20] JLQCD, S. Aoki et al., (2003), hep-lat/0305024,
- [21] JLQCD, S. Aoki et al., Phys. Rev. **D68**, 054502 (2003), hep-lat/0212039,
- [22] A. Duncan, E. Eichten, J. M. Flynn, B. R. Hill, and H. Thacker, Nucl. Phys. Proc. Suppl. 34, 444 (1994), hep-lat/9312046,
- [23] T. Kaneko, Nucl. Phys. Proc. Suppl. **106**, 133 (2002), hep-lat/0111005,
- [24] J. L. Goity, Phys. Rev. D46, 3929 (1992), hep-ph/9206230,
- [25] F. Di Renzo and L. Scorzato, JHEP **02**, 020 (2001), hep-lat/0012011,
- [26] H. D. Trottier, N. H. Shakespeare, G. P. Lepage, and P. B. Mackenzie, Phys. Rev. D65, 094502 (2002), hep-lat/0111028,
- [27] F. Di Renzo and L. Scorzato, (2004), hep-lat/0408015,
- [28] C. Aubin et al., (2004), hep-lat/0402030,

- [29] HPQCD, C. T. H. Davies et al., Phys. Rev. Lett. 92, 022001 (2004), hep-lat/0304004,
- [30] C. W. Bernard et al., Phys. Rev. **D62**, 034503 (2000), hep-lat/0002028,
- [31] M. Wingate, C. T. H. Davies, A. Gray, G. P. Lepage, and J. Shigemitsu, Phys. Rev. Lett. 92, 162001 (2004), hep-ph/0311130,
- [32] G. S. Bali and P. Boyle, (2002), hep-lat/0210033,
- [33] G. Burgio, F. D. Renzo, M. Pepe, and L. Scorzato, Nucl. Phys. Proc. Suppl. 83, 935 (2000), hep-lat/9909169,
- [34] ALPHA, J. Heitger and R. Sommer, JHEP **02**, 022 (2004), hep-lat/0310035,
- [35] S. Collins, The mass of the b quark from lattice nrqcd, 2000, hep-lat/0009040.
- [36] G. S. Bali and A. Pineda, Phys. Rev. **D69**, 094001 (2004), hep-ph/0310130,
- [37] H. D. Trottier, (2003), hep-lat/0310044,
- [38] M. A. Nobes and H. D. Trottier, (2003), hep-lat/0309086,
- [39] ALPHA, M. Della Morte et al., Phys. Lett. B581, 93 (2004), hep-lat/0307021,